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A Diffusion-Split Method To Deal With Thermal Shocks Using Standard Linear Tetrahedral Finite Elements

Víctor D. Fachinotti*† and Michel Bellet*

* *Ecole des Mines de Paris, Centre de Mise en Forme des Matériaux (CEMEF), UMR CNRS 7635, Sophia Antipolis, France*
† *Argentine Council for Scientific and Technical Research (CONICET)*

Abstract. The thermal analysis using linear standard tetrahedral finite elements may be affected by spurious local extrema in the regions affected by thermal shocks, in such a severe way to directly discourage the use of these elements. The present work proposes a slight modification to the discrete heat equation in order to obtain a system matrix in M-matrix form, which assures an oscillation-free solution. The performance of this method is evaluated by means of test case with analytical solution, as well as an industrial application, for which a well-behaved numerical solution is available.

INTRODUCTION

The Galerkin (standard) version of the finite element method (FEM) applied to diffusion problems, when used with linear tetrahedral (P1) elements, does not in general satisfy the maximum principle [1][2][3]. Physically, this principle guarantees to obtain the maximum/minimum of the solution only at the initial time or at the boundary, in the latter case a flow from/to the outside must exist [1]. In thermal analysis, the violation of this principle explains the presence of oscillations in the FEM solution inside the regions affected by thermal shocks, i.e., steep variations of the thermal gradient. These oscillations have been attributed to the mathematical model having physically unrealistic initial conditions [4], which introduces a sudden jump in the solution at the start of the computation. Then, by applying gradually the initial conditions, the modeling of thermal shocks is not longer necessary. But in many important applications processes, such as welding, hot forming and casting, thermal shocks really exist and must be modeled.

The proper modeling of thermal shocks at a given time instant is achieved provided the layer currently affected by the thermal shock be at least one-element wide [5]. This is the so-called penetration depth condition. Therefore, in a purely thermal analysis, thermal shocks have a relatively short-term effect, since the solution is no longer affected once the thermal shock layer is developed enough. However, in a coupled analysis, e.g. a thermo-mechanical analysis, the instabilities caused by thermal shocks in the early stages may invalidate the whole solution, as it is the case for inelastic (history-dependent) materials with thermo-dependent mechanical properties. We can also satisfy the penetration depth condition by refining the mesh in the concerned regions. In metal casting, an initially extremely rapid cooling process takes place at the interface between the melt and the chilled mould, requiring a highly refined mesh on both sides. In 3D, the computational cost implied by such refined meshes in multi-domain problems makes the option of mesh refinement unaffordable.

Let us outline then the different approaches developed to deal with thermal shocks using P1 elements and avoiding mesh refinement.

The first one arises naturally from the penetration depth condition: if the mesh must keep unchanged, a high enough time step, say Δt_{ts}, is needed in the early stage of the simulation. Then, an implicit time-stepping scheme allows to solve the heat equation using Δt_{ts} as time step without stability concerns. Unfortunately, Δt_{ts} is frequently too large for an accurate integration of the heat equation and all the

other conservation equations that may be coupled with it, e.g., the momentum and chemical species balances. Jaouen [6] has proposed to adopt Δt_{ts} as time step, and then to linearly interpolate the computed thermal solution to an adequate time step $\Delta t<\Delta t_{ts}$. This strategy, called asynchronous thermal analysis, gives satisfactory results for linear or slightly non-linear problems, which is not the case in solidification processes.

The second approach is based on the M-matrix theory [7]: the satisfaction of the maximum principle requires the system matrix obtained after discretization be an M-matrix[1]. Putti and Cordes [1][2] proposed an Orthogonal Subdomain Collocation (OSC) technique that produces a diffusion matrix in M-matrix-form when applied to P1 finite elements in a 3D Delaunay triangulation satisfying suitable conditions on the elements geometry adjacent to the boundary affected by thermal shocks. By lumping the capacitance matrix, it becomes an M-matrix. If the capacitance matrix is lumped, it becomes an M-matrix. In such a way, the system matrix for a transient diffusion problem, being the sum of two symmetric M-matrices, is also an M-matrix. It is not longer the case when the system matrix contains an advection (non-symmetric) term, and therefore this approach can not be generalized to advection-diffusion problems. In addition, the geometrical constraints on the mesh prevent from using general Delaunay meshing codes. This leads Kosik et al. [3] to directly discourage the use of P1 finite elements, promoting the use of the finite volume method (FVM). However, we can not ignore the wide diffusion of FEM in the existing codes, as well as its versatility compared to FVM.

Not only FVM but also some FEM models are free of oscillations under thermal shocks. This is the case of Taylor-Galerkin discontinuous (TGD) models. In CEMEF, Pichelin [8] and Batkam [9] have developed explicit and implicit TGD models, respectively, to solve thermal problems on general 3D triangulations. They used P0 elements, i.e., tetrahedra with constant temperature inside. Therefore, the use of these techniques implies no more nodal but elemental unknowns. Let us remark that in a typical 3D triangulation, the number of elements is about 5-times greater than the number of vertex nodes. In other words, TGD-P0 elements are not only less convenient than P1 elements in terms of the order of the discretization error, but also regarding the computational cost.

[1] A real, non-singular $n\times n$-matrix $\mathbf{A}=(a_{ij})$ is an M-matrix if $\mathbf{A}^{-1}\geq 0$ and $a_{ij}\leq 0$ for $i\neq j$, $1\leq i,j\leq n$.

The present work aims to retain the advantages of using P1 finite elements, making possible at the same time to model thermal shocks when small enough time increments are used. The diffusion-split method presented here has common items with that of Jaouen [6] regarding the idea of satisfying the penetration depth condition, as well as with those inspired on the M-matrix theory [1][2] that focus on the form of the system matrix. The resulting formulation, representing just a slight modification to the standard Galerkin one, can be easily implemented into existing FEM codes.

THE HEAT EQUATION

The well-known local form of the heat equation is

$$\rho c_p \frac{dT}{dt} - \nabla \cdot (k \nabla T) = Q \quad \text{in } \Omega \qquad (1)$$

where Ω is the analyzed domain, t the time variable, T the temperature, ρc_p the specific heat, k the thermal conductivity, and Q an internal heat source. Equation (1) is subject to the initial condition:

$$T = T^0 \qquad \text{at } t = 0 \qquad (2)$$

and the following boundary conditions :

$$T = T_w \qquad \text{on } \Gamma_T \qquad (3)$$

$$-(k \nabla T) \cdot \mathbf{n} = q_w \qquad \text{on } \Gamma_q \qquad (4)$$

$$-(k \nabla T) \cdot \mathbf{n} = h(T - T_{ext}) \qquad \text{on } \Gamma_c \qquad (5)$$

prescribing the temperature T_w on Γ_T, the heat flux q_w through Γ_q, and the heat exchange through Γ_c due to convection to the environment at temperature T_{ext} with h as film coefficient; Γ_T, Γ_q, and Γ_c are non-overlapping portions of the boundary Γ of Ω, being $\mathbf{n}$ the unit normal vector pointing outwards to Γ.

Standard Finite Element Formulation

The Galerkin FEM applied to the initial and boundary value problem defined by equations (1) to (5) yields the system of first-order differential equations (see the classical FEM literature, e.g. [4], for details)

$$\mathbf{C}\frac{d\,\mathbf{T}}{dt}+\mathbf{K}\mathbf{T}-\mathbf{F}=\mathbf{0} \qquad (6)$$

where **T** is the vector of nodal unknown temperatures**,** **C** is the capacitance matrix, **K** the conductivity matrix, and **F** is the internal source and external flux vector, defined as

$$C_{ij}=\int_{\Omega}\rho c_p N_i N_j dV \qquad (7)$$

$$K_{ij}=\int_{\Omega}k\nabla N_i\cdot\nabla N_j dV+\int_{\Gamma_c}hN_i N_j dS \qquad (8)$$

$$F_i=\int_{\Omega}QN_i dV+\int_{\Gamma_c}q_w N_i dS+\int_{\Gamma_c}hT_{ext}N_i dS \qquad (9)$$

being N_i the shape function associated to node i. The fully-implicit Euler-backward scheme is used to integrate equation (6) in the time space. Then, once the temperature at time t, say $\mathbf{T}^t$, is known, the temperature **T** at time $t+\Delta t$ can be obtained by solving the discrete equation

$$\mathbf{C}\frac{\mathbf{T}-\mathbf{T}^t}{\Delta t}+\mathbf{K}\mathbf{T}-\mathbf{F}=\mathbf{0} \qquad (10)$$

THE DIFFUSION-SPLIT METHOD

For a mesh of uniform element size Δx, the time increment Δt_{ts} required to satisfy the penetration depth condition, and hence to model properly thermal shocks, is given by

$$\Delta t_{ts}=\alpha\frac{\rho c_p}{k}\Delta x^2 \qquad (11)$$

where α is a constant of order 1 [5].

Further, we know that the spurious solutions observed in case of thermal shocks are associated to the form of the system matrix [1][2][3]. Then, let us rewrite the governing equation (10) by splitting the diffusion term as follows

$$\mathbf{C}\frac{\mathbf{T}-\mathbf{T}^t}{\Delta t}+\mathbf{K}^*\mathbf{T}-\mathbf{F}=\mathbf{S} \qquad (12)$$

where

$$\mathbf{S}=(\mathbf{K}^*-\mathbf{K})\,\mathbf{T} \qquad (13)$$

$$K^*_{ij}=\int_{\Omega}k^*\nabla N_i\cdot\nabla N_j dV+\int_{\Gamma_c}hN_i N_j dS \qquad (14)$$

Now, assuming **S** to be an explicit source term, an augmented conductivity k^* can be defined to satisfy the penetration depth condition for Δt as the first time step:

$$k^*=\begin{cases}k & \text{if } \Delta t_{ts}\le\Delta t\\ k\dfrac{\Delta t_{ts}}{\Delta t} & \text{if } \Delta t_{ts}>\Delta t\end{cases} \qquad (15)$$

The value of k^* decreases with time from the value given by equation (15) at t=0 to the real conductivity k when $t+\Delta t\ge\Delta t_{ts}$. Therefore, in the latter case, equations (10) and (13) are identical. Regarding the source term **S**, an explicit approximation is built by taking a known value of **T** in equation (13), $\mathbf{T}^t$ being the best choice since any approximation to **T** obtained using an explicit time-stepping scheme may be affected by instabilities. Thus,

$$\mathbf{S}\approx(\mathbf{K}^*-\mathbf{K})\,\mathbf{T}^t \qquad (16)$$

It is interesting to note that during the early stages of the simulation, there is no sensible variation of the temperature outside those regions under thermal shocks, and hence the approximation implied by equation (16) is local and temporary.

The Penetration Depth Condition On Unstructured Meshes

For non-uniform unstructured meshes, the computation of Δt_{ts} using equation (11) complicates due to the uncertain definition of the mesh size Δx. Jaouen [6] explores all the non-adiabatic boundaries of the analyzed domain, determining the minimum, the maximum, and the average value of Δx, the choice of the adequate value left to one's expertise. Being the square value of Δx involved in equation (11), the influence of this choice on the proper modeling of thermal shocks is crucial. In practice, Δt_{ts} is underestimated when computed with the minimum Δx, and hence the penetration depth condition is not satisfied. On the other hand, the use of the maximum Δx, leading to an overestimation of Δt_{ts}, has a detrimental effect on the accuracy of the diffusion split method, producing an excessively large k^*. Using the average mesh size, the result is uncertain.

If it were possible to identify a priori those regions under thermal shocks, and the mesh within each region were quite uniform, then we could define a different Δt_{ts} (and hence a different k^*) for each region. Anyway, for the sake of simplicity, we prefer to determine a global Δt_{ts}. In case of monotonic cooling, Δt_{ts} can be easily determined by solving equation (12) for increasing Δt_{ts} until the computed temperature not exceed the previous one at each node of the mesh. This should not take more than a few iterations to obtain an accurate enough value of Δt_{ts}. Normally, this is made only once at the beginning of the simulation, so the additional computational cost is negligible in practice.

THE DIFFUSION-SPLIT METHOD FOR SOLIDIFICATION PROBLEMS

In case of liquid-solid phase change, we introduce the enthalpy function

$$H(T) = \int_0^T \rho c_p(T) dT + g_l \rho L \qquad (17)$$

where g_l is the mass fraction of liquid ($0 \le g_l \le 1$, $g_l=0$ in the solid, $g_l=1$ in the liquid), assumed to be a given function of the temperature, and L the specific latent heat of solidification. Let us assume the existence of the function $T=T(H)$, inverse of that given by equation (17). Then, we can rewrite the heat equation (1) with the enthalpy as the primal variable:

$$\frac{dH}{dt} - \nabla \cdot \left[k \nabla T(H) \right] = Q \quad \text{in } \Omega \qquad (18)$$

subject to the initial condition (2) and the boundary conditions (3) to (5). After using Euler-backward scheme for time discretization and FEM for spatial discretization, we obtain the discrete heat equation:

$$\mathbf{C} \frac{\mathbf{H} - \mathbf{H}^t}{\Delta t} + \mathbf{K}\mathbf{T} - \mathbf{F} = \mathbf{0} \qquad (19)$$

where **H**, the vector of nodal enthalpies, is the current unknown, the temperature at each node i being a dependent variable: $T_i=T(H_i)$. The diffusion matrix **K** and the external flow vector **F** are those already defined, equations (8) and (9), respectively, while **C** is now the typical mass matrix

$$C_{ij} = \int_\Omega N_i N_j dV \qquad (20)$$

Equation (19) is usually highly non-linear for solidification problems, and is solved using the Newton-Raphson iterative technique.

The procedure to apply of the diffusion-split method in this case is identical to that previously described. It yields

$$\mathbf{C} \frac{\mathbf{H} - \mathbf{H}^t}{\Delta t} + \mathbf{K}^* \mathbf{T} - \mathbf{F} = (\mathbf{K}^* - \mathbf{K}) \mathbf{T}^t \qquad (21)$$

Now, rather than the specific heat ρc_p, it is an effective heat capacity ρc_{eff} accounting for the latent heat evolution that enters in the definition of the time step Δt_{ts}, equation (11). In the elements undergoing phase change, ρc_{eff} is considerably greater than ρc_p. Also, it is highly variable with time. These facts make not always valid the a priori estimate of Δt_{ts}. It can be valid in solidification processes where the initial temperature is not too close to the liquidus temperature. Anyway, Δt_{ts} should be determined at each time step until thermal shocks effects completely disappear. Actually, a general and efficient procedure to determine Δt_{ts} for non-linear problems and unstructured meshes remains a research item.

APPLICATIONS

Test Case I: One-Dimensional Cooling

Let us consider first the one-dimensional case of a semi-infinite domain, initially at the uniform temperature $T^0=800^oC$, whose surface temperature suddenly falls to a value $T_w=25^oC$, kept constant. Table 1 lists the material properties. This problem illustrates some typical features of thermal analysis in steel hot forming. We use a structured finite element mesh with uniform element size Δx = 2 mm in the flux direction. A constant time step Δt=0.1 s is adopted.

In this case, the original Galerkin solution is affected by thermal shocks, as evidenced by the spurious temperature increment of 13.2°C at the first time step for a node located 4 mm-far from the cooled wall (Figure 1). For linear tetrahedral finite elements and consistent (not-lumped) capacitance matrix, the constant α in equation (11) is taken equal to unity [6], obtaining then Δt_{ts}=0.748 s. However, using the procedure described in the preceding section, every nodal point is already free of unphysical heating for Δt_{ts}=0.544 s. And, by tolerating a small temperature

increment of 0.1°C for instance, this value reduces to 0.287 s. The augmented conductivity k^* is computed using equation (15) for the first time step, and decreases linearly with time until reach the original value k for $t \geq \Delta t_{ts}$. Let us remind that the closer the values of Δt and Δt_{ts}, the lesser the artificial increment of the conductivity in the thermal regions when the diffusion split method is used. This is clearly evident in Figure 1 where the temperature rate at the first time step increases with as k^* does, which is an unphysical but numerical effect of diffusion split method.

TABLE 1. Material properties for test case I

Density ρ	7800 kg/m^3
Heat capacity c_p	360 J/(kg°C)
Thermal conductivity k	15 W/(m°C)

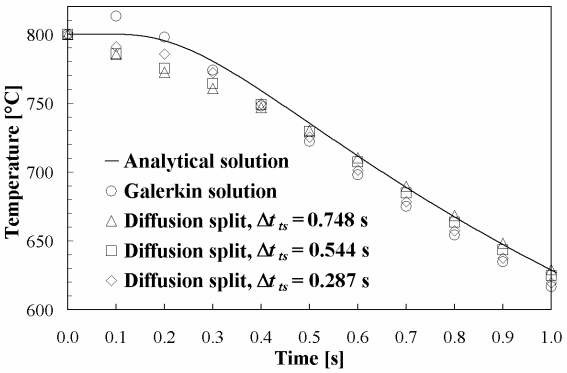

FIGURE 1. Early evolution of the temperature at node situated 4 mm-far from the chilled wall.

Test Case II: Ingot Solidification

We consider now the ingot casting model shown in Figure 2. The material properties of each component and other model parameters are listed in Table 2. The model is axisymmetric, and a small sector of 12° is considered for 3D simulation. The ingot has a radius of 0.433 m at the top, an its total height is 2.58 m. This is a typical simulation illustrating the problems posed by thermal shocks in current 3D applications. First, due to the very different diffusion properties of the different parts, an excessively large time step is needed in order to satisfy the penetration depth condition. Taking into account the average element size (since the mesh density is quite uniform in each subdomain), equation (11) yields the values of Δt_{ts} listed in Table 2.

For Δt=0.1 s (an adequate value of the time increment for the early stages of the simulation), the obtained using standard Galerkin FEM with P1 elements is completely useless, exhibiting nodal temperatures that are 94°C above the initial temperature in the ingot. The solution is even worse in the domain of smaller diffusivity: in the powder, this spurious overheating attains 320°C, while negative temperatures are observed in the insulating domain.

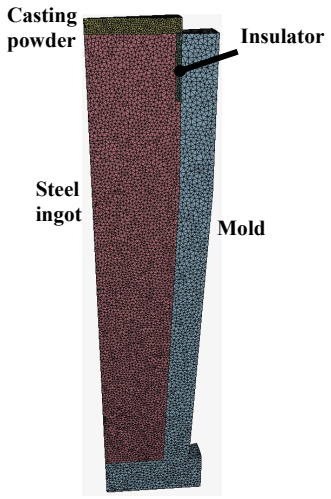

FIGURE 2. FEM model of an ingot casting process.

TABLE 2. Model data for test case II.

Ingot	
Density ρ	7450 kg/m^3
Heat capacity c_p	510 J/(kg°C)
Thermal conductivity k	30 W/(m°C)
Latent heat L	241000 J/kg
Solidus temperature	1432°C
Liquidus temperature	1454°C
Initial temperature	1534°C
Time step Δt_{ts}	20.3 s
Mould	
Density ρ	7200 kg/m^3
Heat capacity c_p	600 J/(kg°C)
Thermal conductivity k	30 W/(m°C)
Initial temperature	80°C
Time step Δt_{ts}	36.3 s
Insulator	
Density ρ	780 kg/m^3
Heat capacity c_p	848.5 J/(kg°C)
Thermal conductivity k	0.82 W/(m°C)
Initial temperature	60°C
Time step Δt_{ts}	41.3 s
Casting powder	
Density ρ	500 kg/m^3
Heat capacity c_p	1100 J/(kg°C)
Thermal conductivity k	0.35 W/(m°C)
Initial temperature	1534°C
Time step Δt_{ts}	70.3 s
Interfaces	
Contact thermal resistance	0.001 m^2°C/W

In order to apply the diffusion-split solution, we choose to admit an overheating of 0.5°C in the ingot at the first time step. In such a way, the value of Δt_{ts} falls

to 11 s, and considerably less artificial diffusion is added. A reference solution is obtained using the implicit TGD method with P0/P0$^+$ triangular elements [9], probed to be free of the instabilities caused by thermal shocks. Figure 3 shows the temperature through a cross section of the ingot, situated 1.60 m far from the bottom, at the beginning of simulation (t=1.1 s). A good accord between diffusion-split and TGD solutions is observed. The points in the plot correspond to the center of the TGD elements, while they are nodal values for the 3D triangulation, letting us note that the TGD mesh is about 2.5-times denser than the 3D mesh in this region. Once the solidification has progressed in the ingot, the agreement between both models remains satisfactory, as evidenced in Figure 4 for the temperature at t=2 h.

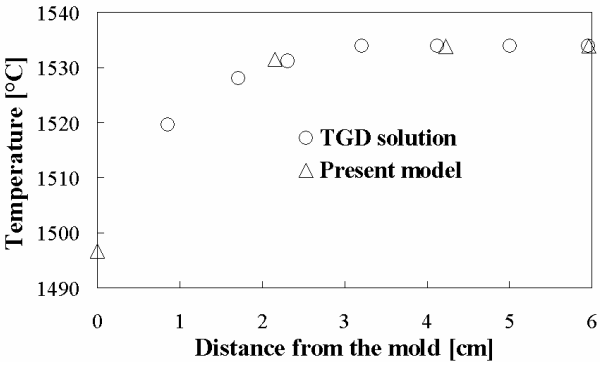

FIGURE 3. Temperature in the ingot at 1.1 s in a cross section located 1.6 m-far from the bottom.

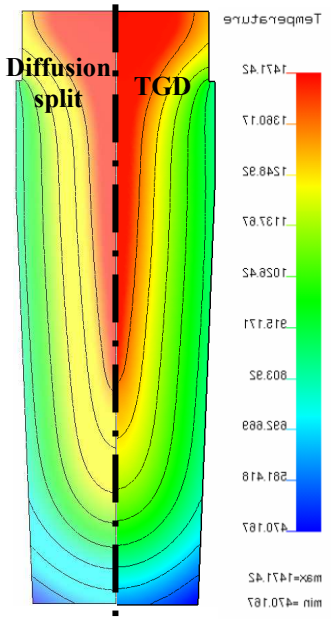

FIGURE 4. Temperature in the ingot after 2 hours of solidification.

CONCLUSIONS

The diffusion-split method makes possible to solve problems involving thermal shocks using the FEM with P1 tetrahedral elements. Compared to the previous models using P1 elements, the diffusion split method works for general meshes, contrary to the OSC-FEM method [1][2], and the heat equation is solved for an adequate time step (i.e. not excessively large), contrary to the asynchronous analysis [6]. Compared to the TGD method using P0$^+$/P0 elements [9], the present model has not only a better accuracy order, but also a smaller computational cost. The present model can be implemented in most existing FEM codes with a minimal effort.

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